NEWSLETTER

Society of Crystallographers in Australia and New Zealand

http://www.sca.asn.au/

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FROM THE PRESIDENT

Happy 2014, the International year of Crystallography! I hope everyone had great Christmas holidays, and I wish you a smooth return to work. For many of us the grant application deadlines are looming again, but it is nice to see sanity returning to the ARC, with the Discovery Project restrictions lifted for those who hold NHMRC funding.

Thanks to Charlie Bond, two very important things happened in the recent months relevant to SCANZ members communication. First, we have a beautiful new website, http://scanz.iucr.org/, please check it out and let us know what you would like to be added or changed on it. Second, we have the [SCANZ-info] mailing list, which is a self-subscription mailing list for emails discussing anything relevant to SCANZ members, including crystallographic issues, employment opportunities, equipment and expertise requests. The list is rather useless unless most members join, so please do so as soon as you can, the instructions are on SCANZ website.

WE ARE:

From the President

The most pressing thing is to remind everyone that the Crystal-29 conference is not far away, and abstract submission, award nomination and registration deadlines are approaching. Please visit www.crystal29.com and I hope to see many of you in the South-East Queensland rainforest.

The triennial International Union of Crystallography (IUCr) Congress is also taking place this year in Montreal, Quebec, Canada. I attended an American Crystallographic Association (ACA) Conference in Montreal about 10 years ago, and it is a great place to visit. Anybody who ever attended an IUCr Congress will tell you it is an essential experience for any crystallographer, because it is the best way to see first-hand the breadth of crystallography going on worldwide. The one held during the International Year of Crystallography should therefore be extra special!

There is in fact some interest in Australia to host an IUCr Congress some time in the future, especially by crystallographers in Melbourne and Sydney. Because of the nature of the bidding process, this really means quite some years in the future, when some of us may be retired or nearing retirement. Two things are therefore essential if going ahead with the bid: some young-ish crystallographers need to be involved, who will actually be around if the bid is successful, and different interested groups in different cities and states need to unite and support one strong bid.

The International Year of Crystallography (IYCr) has now officially started, with the Opening Ceremony taking place 20-21 January in Paris. A few Australians attended this event and Chris Howard has written an account of the experience which is included in this newsletter. A number of activities are being planned around Australia, and I would like to sincerely thank all those who are contributing to these activities. For this special year, SCANZ has ear-marked quite a large amount of funds (considering the usual SCANZ standards) of $20,000 to seed and support various activities. It is not too late for any new ideas, and to help out with any planned activities! We particularly need more early-career researchers involved. Please read more about various activities from the people coordinating them in this Newsletter. Special thanks also to Mitchell Guss as the Chair of the National Committee of Crystallography, and the Australian Academy of Science for lending us Poulomi “Polly” Agrawal, who is helping with the coordination of IYCr activities.

Lastly, a word on IUCr journals. The Union is on a mission to increase the influence of its journals among the wider scientific communities and broaden their scope, so that high-quality science papers incorporating crystallography are attracted to the journals. One of the steps towards these aims is the launch of the new journal IUCrJ. It is an open-access comprehensive journal that is aiming to attract high quality papers of wide scientific significance from all areas that use diffraction methods.

With this year being the International year of Crystallography, it is a perfect time to join SCANZ. Most of us know colleagues who use crystallography but are not SCANZ members. Please encourage your colleagues to join.

Bostjan Kobe, President

Meeting Report AsCA 13

Hong Kong, Dec 7-10, 2013

The Asian Crystallographic Association had an eventful year which culminated with a successful AsCA conference held at the Hong Kong University of Science and Technology (HKUST) from December 7-10. Although the meeting was originally scheduled to be held in Dhaka, Bangladesh, the political instability in that country led the Council to decide to move the venue. Fortunately Professor Ian Williams from HKUST offered to host the meeting at his institution in Hong Kong and, together with the International Program Committee led by Takashi Kamiyama (Japan), an exciting and diverse program consisting of 18 microsymposia was organized in a relatively short time. Approximately 413 attendees were present at the conference and associated symposia and workshops from 30 different countries.

At the AsCA Council meeting elections were held to appoint the new Executive. Professor Pinak Chakrabarti (India) is the new AsCA president and Professor Jennifer Martin (Australia) is the Vice-President. Professor Se Won Suh (Korea) is the Past President and Professor Jagadese Vittal (Singapore) is the Secretary Treasurer.

All AsCA member countries are actively engaged in activities directed at celebrating the International Year of Crystallography. In addition, AsCA is currently focusing on expanding its membership through invitation for more Asian countries to join the Association.

The next AsCA conference will be held in 2015 at the Science City Auditorium, Kolkata, India. The Chair for the Local Organizing Committee is Professor Pinak Chakrabarti and the Chair for the International Program Committee is Professor Alice Vrielink. The meeting will be held from December 5 – 8, 2015.

By Alice Vrielink
(AsCA Secretary/Treasurer (2010 – 2013)

AsCA 13, Maslen Scholarship Reports

The 2013 Asian Crystallographic Association Meeting (AsCA'13) was held at the beautiful campus of Hong Kong University of Science and Technology. Among the regional associates of International Union of Crystallography (IUCr), AsCA is said to be the youngest and fastest growing. This meeting of course attracted a large group of attendees from Asia-Pacific region and also from all over the world. As a follow-up of the AsCA/ SCANZ joint meeting and Bragg Symposium last year in Adelaide, SCANZ has played an important role in the organization of the AsCA meeting, and also been well presented by the attendees from Australia and New Zealand. Thanks to the Maslen Scholarship from SCANZ, I was grateful to be one of the lucky students to attend this meeting.

The meeting was preceded by the South China Structural Biology Symposium, which started with a keynote lecture by Prof Peter Colman from WEHI and showcased the crystallographic research going on in South China area. This symposium was very inspiring for me as a Chinese student who is studying crystallography in Australia.

The following AsCA meeting was well organized and covered a wide range of topics in crystallographic research. These topics were classified into microsymposia covering applications of crystallography in life sciences and chemical materials, incorporating synchrotron and neutron studies. As a prelude to the International Year of Crystallography (IYCr2014), the AsCA meeting also featured many lectures to promote this event.

There were too many great talks to mention. Alice Vrielink talked about their challenging work on a membrane protein involved in the antibiotic resistance of the superbug Neisseria, which gave us insights into the resistance mechanisms and provides potential strategies for future drug design. Amit Sharma drew a huge map of macromolecular assemblies consisting of histone, DNA and NAP proteins in Malaria pathogenesis. My supervisor Bostjan Kobe gave a very entertaining presentation about the "spring-hammer" mechanism of Streptococcus protein PsaA.

It was interesting to see how crystallography is used in very different fields from my own. Mike Zaworotko gave an excellent plenary lecture on crystal engineering of task-specific materials. I was impressed that they could name their new materials after the student working on the project. An overview of history and exiting developments of synchrotron facilities and neutron sources was given in Sine Larsen's talk.

In addition to the oral and poster presentations, there were workshops and industry stalls for crystallographic software and databases. The delegates from the CCP4 developing team gave me useful advice on using the software. Ronan Keegan especially helped me find a MR solution for one of my datasets that has been a very hard case.

I was honored to receive the Rising Star Award for young scientists and presented my work on plant disease resistance proteins and fungal effector proteins in the meeting. I received much positive feedback for my talk and it has been a great experience for me.

Xiaoxiao Zhang

University of Queensland

AsCA 13, Maslen Scholarship Reports

The 12th meeting of the Asian Crystallographic Association (AsCA '13) was held in December last year at the picturesque Hong Kong University of Science and Technology campus. The conference was well represented with scientists not only from Asia-Oceania, but also from around the world. A series of lectures were given, encompassing broad crystallographic topics ranging from hot structures in biology, chemical crystallography to various new diffraction techniques.

I particularly enjoyed the talk given by Dr Kenichi Kato on the conversion of property of layered oxide from electronic conductor into superionic conductor. Although, a special mention should be given to Prof Brendan Kennedy, who cleverly incorporated the "more than one way to skin a cat" phrase to explain pyrochlore-fluorite transformation.

I was really honoured to receive the Rising Star award, as it was a chance for me to present my PhD project in front of a wide scientific audience. It was definitely a daunting and yet satisfying experience.

One of the highlight of AsCA 13 was the conference dinner, held at the famous Jumbo Kingdom floating restaurant in Aberdeen harbour. It was a chance to mingle with fellow students and all the local and international speakers. As we enjoyed the banquet, serenaded by the beautiful music emanating from guzhengs (Chinese zithers), we celebrated another successful conference.

Finally, I would like to take this opportunity to thank SCANZ for the Maslen scholarship, allowing me to attend the AsCA '13 conference.

Denissa Murphy
The University of Sydney

It was a great privilege to be awarded the Maslen scholarship to attend the AsCA 13 meeting in Hong Kong. The conference was extremely well organised and provided the chance for me to see presentations of some of the most cutting edge science involving crystallography. I was also able to discuss and learn from leading scientists through presenting a poster of some of the work from during my PhD candidature.

Each micro-symposium catered to a variety of interests from chemical structures, to materials and to the biological sciences. Prof. Mike Zaworotko's opening plenary was particularly interesting, I think, to all, and helped build a sense of excitement for the duration of the conference. This is the science that will lead tomorrow.

As a post-graduate student I could not write a true reflection of my experiences at the conference without at least briefly mentioning the conference banquet at the floating Jumbo Kingdom restaurant. There was a full fare of local delights in a fantastic environment to meet other students and researchers.

Attending AsCA was truly a valuable learning experience and I would like to sincerely thank SCANZ for the opportunity to attend, and also thank the conference organisers.

Thomas Godfrey,
The University of Sydney

The Jumbo Kingdom Floating restaurant, the venue for the conference dinner

Special thanks to Bill Duax for photos of ASCA13

Launch of the International Year of Crystallography – Opening Ceremony UNESCO House, Paris, 20-21 January 2014.

by Chris Howard

After a few days in Cambridge to combat jetlag, I crossed the channel by Eurostar on the afternoon of Saturday 18th January. This gave me a free day in Paris on Sunday. Paris is known as a city of lovers, but I saw that on Sunday morning it was much more a city of joggers – along the banks of the Seine, through the gardens, wherever I ventured. I looked hard to recognise other crystallographers, especially around the UNESCO centre and in my hotel, but without success. There was no evidence that crystallographers were taking over this part of the city, and I wondered how many would attend.

On Monday morning I was to find the answers to some of my questions. Suits were not out of place. At registration we were issued tags, but these were not name tags, and there was no participants list. I found this disappointing, and was to learn at the end that arrangements were made late due to doubts about the meeting's funding. I looked for Australians in attendance, and found Peter Colman, Richard Garrett, Mitchell Guss and Shane Kennedy, along with expatriate Australians Sax Mason (Institut Laue-Langevin) and John Spence (Arizona State).

Monday's sessions were particularly well attended, with the lecture theatre, said to hold 800, not far from full.

The Monday morning audience

The first session was a collection of welcoming remarks – a recorded video welcome from Ban Ki-moon (who was probably busy sorting out Syria on the day), an address from the UNESCO Director-General who formally opened the meeting, then further welcoming speeches from the President and Vice President of the International Union of Crystallography (IUCr), a representative of the Moroccan government (that Kingdom put the case to declare 2014 as IYCr), the President of the Centre National de la Recherche Scientifique (CNRS), and Presidents or Past Presidents of the International Union of Pure and Applied Chemistry, European Physical Society, International Mineralogical Association, and the International Union of Biochemistry and Molecular Biology. Some of these talks recognised that 2011 was the International Year of Chemistry and 2015 will be the International Year of Light. There were remarks on the history of crystallography, and on the history of IUCr, and the UNESCO speakers seemed to show particular interest in the contribution that crystallography might make to sustainable development. I lost some of this (from the native French speakers) because it took me some time to work out the interpreter service. The IUCr Vice-President described the IUCr-UNESCO program of Open Labs in Africa, South and Central America, and South Asia.

Following coffee Jenny Glusker talked on the history of crystallography, including very early speculation (e.g. by Robert Hooke, 1665) that the regularity of crystal forms must imply a regular arrangement of the internal constituents. Of course the history of crystallography since the discovery of X-ray diffraction is more familiar to most of us, and Jenny took us through the usual highlights in a most professional manner. Immediately after this there was a session entitled 'Talented young crystallographers of the world' chaired by freelance science writer Philip Ball. In his introductory remarks Philip dipped into history a few times – showed William Bragg and Max von Laue together at a Solvay Conference in Brussels in 1913 (however national rivalries were apparent at that time), mentioned the history of success of women crystallographers (for example Hodgkin, Lonsdale, Franklin), and remarked on a recent high-resolution study (Umena *et al.*, Nature, 2011) that throws light on the splitting of water at the membrane-protein complex photosystem 2. Then eight 'talented young crystallographers' – not all so very young and mostly well established – gave their presentations by pre-recorded video. They sat on stage along with a similar number of perhaps younger and less well established crystallographers, and after the videos engaged in discussion under Philip Hall as chair. They raised familiar issues – short period funding, intense pressure on young scientists to teach and

'Talented Young Crystallographers' in Paris

publish – as well as issues relating to lack of resources in some countries and the difficulty of pursuing unequal collaborations.

After lunch we moved from young crystallographers to a Nobel Laureate. After training as a physician, Brian Kobilka realised that crystallography would enable him to 'see' his favourite molecules. His interest is the system of message transmission through cell walls. This involves a stimulant (agonist) outside the cell, a receptor that is embedded within the membrane, and a protein inside the cell wall. The protein is known as a G-protein, and the receptor as a G-protein-coupled receptor. He shared the Chemistry Prize in 2012 for his high resolution crystallographic studies of the active ternary complex comprising the agonist, the β2-AR (andrenergic – i.e. responsive to adrenaline) receptor, and the G-protein. The work was challenging at every turn – extraction of complex from membrane, expression, purification, crystallisation – the diffraction studies at the APS and ESRF, and the need for tricks such as the use of antibodies to stabilise the conformation. The crystallography suggests that the action of the agonist on the receptor is amplified through the membrane by the receptor geometry. The structural details of the receptors are of great pharmaceutical interest because they are often the targets for drugs. Comments were made on both the years devoted to the project, and the extent of collaboration involved.

The final session on Monday was given to a review of crystallography in the BRICS countries – Brazil, Russia, India, China and South Africa. I had not previously encountered this grouping, and am not sure of the basis for it. In opening remarks, UNESCO reiterated hopes that crystallography might provide a vehicle for promoting sustainable development, for encouraging women into science, and for north-south collaboration. The BRICS countries were represented variously by ambassadors, government science bureaucrats, and crystallographic association chairs. A number of these countries appeared to be persuaded of the nexus between scientific research and economic growth – I am unsure that the Australian government is persuaded of such a link – and were increasing their investments accordingly. Brazil in particular was ramping up science support as a fraction of GDP, had 7.2 million students enrolled in tertiary education (maybe not just science), 13th in publication output, with increasing citation impact. This investment was considered to have enhanced activities in petroleum industry, aerospace (3rd in world), and agriculture (Brazil now net exporter). Brazil is also a leader in the use of bioethanol for vehicle fuel. Brazil established the first synchrotron radiation source in the southern hemisphere in 1997, and was building its second synchrotron to come on line in 2016. It was claimed Brazil has 3,000 Ph.D. crystallographers. It will play a leading role in the recently established Latin American Crystallographic Association. South African crystallography started in 1937 in Capetown with R.W. James (who had worked with Bragg), then developed through his students, and his students' students. Evidently quite strong in supramolecular chemistry, but short on macromolecular crystallography, which I would attribute to lack of access to synchrotrons. India also has a good tradition in crystallography, again with an emphasis on supramolecular chemistry and crystal engineering, with some good protein crystallography but that perhaps limited by limited access to synchrotrons. I am moved to reflect that protein crystallography in Australia benefitted from good arrangements for synchrotron access well before the commissioning of the synchrotron in Melbourne. Russia has great traditions dating back to the 19th century, while China has been opening up its activities (e.g. two-way traffic of scientists) as well as constructing new facilities. Current Chinese activities encompass metal-oxide-framework systems, molecular ferroelectrics, molecular nanomagnets and, in the macromolecular field, the structures of light harvesting proteins and the SARS virus.

John Spence on X-ray lasers

On Tuesday the meeting more closely resembled the usual scientific meeting – suits no longer required. John Spence (Arizona State) opened with a fascinating talk on X-ray lasers and their use in crystallography. These give very short (femtosecond) pulses of great intensity. The breakthrough realisation was that while one pulse was guaranteed to destroy any crystal, the process of destruction was so slow that the pattern could be captured before this occurred. The strategy is one of 'diffract then destroy.' Data are collected by directing the X-rays through a jet containing tiny crystals. There is the possibility of obtaining X-ray patterns from single particles, such as viruses – with this technique the phase problem might be circumvented. A current interest is the study of photosynthesis by time-resolved

crystallography. Martijn Fransen (PANAlytical) brought us back onto laboratory scale, with a review of the impact of (mostly powder) X-ray diffraction in the cement industry, ore analysis, pharmaceuticals, microelectronics, and crystal deformation. Juliette Pardon (CCDC) spoke on research involving collaboration between CCDC and a group in the University of Kinshasha (DRC) – this involving two way visits of students and staff. David Bish (Indiana) and David Blake (NASA) gave an account of research carried out using the (very) portable X-ray diffraction (XRD) / X-ray fluorescence (XRF) device, developed over twenty years, and now carried on Mars by the Curiosity rover. It returned its first X-ray diffraction patterns in October 2012. The first analysis from a sand dune showed amorphous content, no hydrated minerals, no clay, feldspar, and was generally similar to the basaltic soil found on the flanks of the Mauna Kea volcano in Hawaii. The second sample was from a drilling rig – this now contained both clay minerals and a hydrated mineral, bassanite. Mars is now a dry environment, but it seems it was wet in the past. The next talk was from Frank Burgazy (Bruker) on the history of crystallographic technology. He covered X-ray tubes (first commercial tube produced by Siemens just three months after Roentgen's discovery), optics, detectors, and software. The latest laboratory X-ray source is based on a liquid metal jet, as a means to overcome the problem of power dissipation. The final talk in the pre-coffee session was from Philippe Walter (CNRS, Paris) on the applications of X-ray diffraction in the study of art and historical artefacts. The approaches are to take a very tiny sample, when permissible, for evaluation at a synchrotron, or to take a portable X-ray diffractometer (cf the Mars probe) to the painting or artefact of interest. The studies of art depend on the fact that most pigments are crystalline – e.g. $PbCrO_4$ commonly used for yellow. Can check compositions and also the size and shape of crystallites – da Vinci set down 2 μm layers of glaze. The methods can be used to check authenticity, trace the trade in pigments, and to assist in conservation. I derived some personal satisfaction in seeing that quantitative phase analysis, via the Rietveld method applied to X-ray powder patterns, in the development of which I played some personal part (Hill & Howard, JAC, 1987), was showing up in the laboratory (Fransen), on Mars (Bish) and even in the world of art (Walter).

Captive audience, includes Bill David and Andy Fitch

After coffee, we moved gently from the study of art to art itself, namely Islamic art, firstly in the hands of Abdelmalek Thalal (Marrakech) and Emil Makovicky (Copenhagen). Certain Islamic art is strong on the symmetries of constellations, and of periodic tilings. Many of the tilings have symmetries that can be identified with the plane groups that are reported in our International Tables. There are also instances of quasi-periodic tilings with five or ten-fold motifs. Certain architectural features show an 'under and over' character, and are better described using layer groups (with which I am not familiar). Makovicky showed examples of mistakes in periodic tilings, amounting to twin boundaries and the like – maybe not so surprising if one considers that there would be many workmen involved in the process. Peter Lu (Harvard) gave the final rather mathematical account of Islamic tilings. The building blocks of quasi-periodic Islamic architecture are, he claimed, the five Girih tiles, as appear in the Topkapi scroll. Peter indicated a connection of Girih with Penrose tiles, and finally a connection to the Fibonacci sequence. Fascinating stuff, but it would take me much more time to digest it.

This brought us close to the end of the meeting. Samar Hasnain (Liverpool), Editor-in-Chief of IUCr journals, gave an account of the role of those journals in the international development of crystallography. There followed a talk by Chris Llewellyn Smith (Oxford) on the development in Jordan of an international synchrotron source, SESAME (Synchrotron–light for Experimental Science and Applications in the Middle East). Chris had been Director at CERN, and I learned that CERN had been set up after WW2 by UNESCO in an effort to encourage cooperation between previously warring nations as well as to further science. SESAME will be a 2.5 GeV third generation light source. The current members are Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, the Palestinian Authority and Turkey. The dual purposes of encouraging cooperation between warring nations and furthering science are evident. Maciej Nalecz (UNESCO Basic Sciences) gave a short closing speech.

All in all, an interesting day and a half, and I think worth the hours of travel involved. As to the International Year of Crystallography itself, it behoves all of us to try to make it a success.

Special thanks to Bill Duax for photos of the IYCr opening ceremony

International Year of Crystallography Activities

A number of activities have been planned to celebrate the International Year of Crystallography, contact the organizers of these projects if you wish to help out with any of these activities. Additionally, SCANZ has agreed to support IYCr activities collectively with $20,000. If you have an idea for an activity that you would like supported by SCANZ, please send Chris Ling a short proposal of what you plan to do and what the funds would be used for.

IYCr Photo Competition "Crystallography in Everyday Life" - Jenny Martin

Amateur and professional photographers are invited to submit stunning images that capture the spirit of crystallography in the places, objects and experiences of everyday life. The best images received by March 31 2014 will be exhibited publicly in Australia and will feature at the SCANZ Crystal29 conference (www.crystal29.com) in Queensland. Crystal29 attendees will vote for the "Crystallographer's Choice" Image (prize $500 Australian). All Images received by May 31 2014 will be eligible for the IUCr/Agilent international prize - $USD1000 to attend the IUCr Congress in Montreal in August 2014 and the possibility of featuring in an IUCr calendar. For details on how to enter check out the crystal29 home page www.crystal29.com.

Source: Aboriginal Art & patterning@ http://art-educ4kids.weebly.com/aboriginal-art-and-patterning.html

Source: IYCr; Fruit market

Source: Wikipedia: Patterns drawn outside homes in South India

IUCr

Crystallography in everyday life

PHOTO COMPETITION – AUSTRALIAN SATELLITE

2014 international year of crystallography

Amateur and professional photographers are invited to submit stunning images that capture the spirit of crystallography in the places, objects and experiences of everyday life. The best images received by **March 31 2014** will be exhibited publicly in Australia and will feature at the SCANZ Crystal29 conference (www.crystal29.com) in Queensland. Crystal29 attendees will vote for the "Crystallographer's Choice" Image (prize $500 Australian). All Images received by May 31 2014 will be eligible for IUCr/Agilent international prize - $USD1000 to attend the IUCr Congress in Montreal in August 2014

Find out more and submit your entries at
www.iycr2014.org/participate/photo-competition

IUCr SCANZ Agilent Technologies National Committee for Crystallography
A committee of the Australian Academy of Science

International Year of Crystallography Activities

Crystal growing competition - Jennifer Jones

Three national organizations SCANZ, The Australian Academy of Science and the RACI are supporting the idea of a National Crystal Growing Competition as part of the celebrations for the International Year of Crystallography in 2014. Currently seven states and territories run individual competitions organized or assisted by the appropriate RACI Branches and all have agreed in principle to be part of a National Competition. The plan then is that each state/territory carries out their own competition and then sends their winning entries to be judged to find the national winners. For further information contact Jennifer Jones on jennyjonesdr@gmail.com.

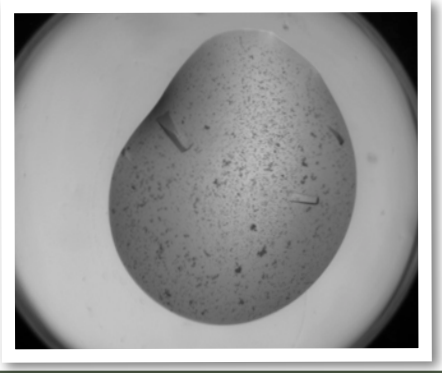
Public display of remote data collection at the Australian Synchrotron - Brett Collins

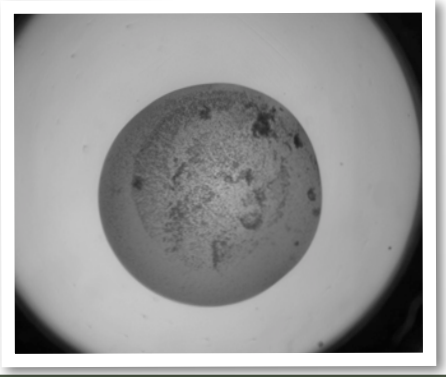
A critical aspect of studying structures of crystals is to use high energy X-rays for diffraction measurements. Australia is fortunate to have the Australian Synchrotron facility that researchers around the country and overseas can use for such experiments. With the advance of robotic technology it is now possible for scientists to perform these experiments remotely from anywhere with an internet connection. In this International Year of Crystallography University of Queensland researchers will demonstrate this approach in an event coordinated by Dr Brett Collins, to show how it is done and to highlight how these experiments are essential for fields as diverse as materials science, evolutionary biology and drug design

Citizen Science Crystal Drop Evaluation - Janet Newman

Janet Newman is leading a proposal to develop a citizen science project for ABC Science's "National Science Week" (http://www.scienceweek.net.au/abc-sciences-national-science-week-citizen-science-project-2014/). Arguably, the hardest part of protein crystallography is producing the sample; but the other hardest part (!) is coaxing that sample into a well-ordered crystal, which will diffract X-rays to a usefully high resolution. The growing use of automation in protein crystallisation has changed the problem – it is relatively easy to set up countless thousands of crystallisation trials, but determining the outcome of the trials is still a process that requires human intervention. Adding a further challenge to this is the unfortunate fact that most of the trials are really not very interesting at all. What would be phenomenally useful would be a robust computer algorithm that could do some of the grunt work of filtering out the subset of crystallisation trials that are interesting enough to require human interpretation.

For this Citizen Science proposal, we will provide lots of images of crystallisation trials, and ask the participants to find a closest match to a set of 10 standard images. Then this data would be used as a training set for a machine learning program. The program would then be able to classify images into sets – some which clearly do not need further analysis, and some which might be interesting to a crystallographer.





With the help of Citizen Scientists, Janet Newman hopes to develop software that can distinguish between drops containing crystals (left image) and those without (right image).

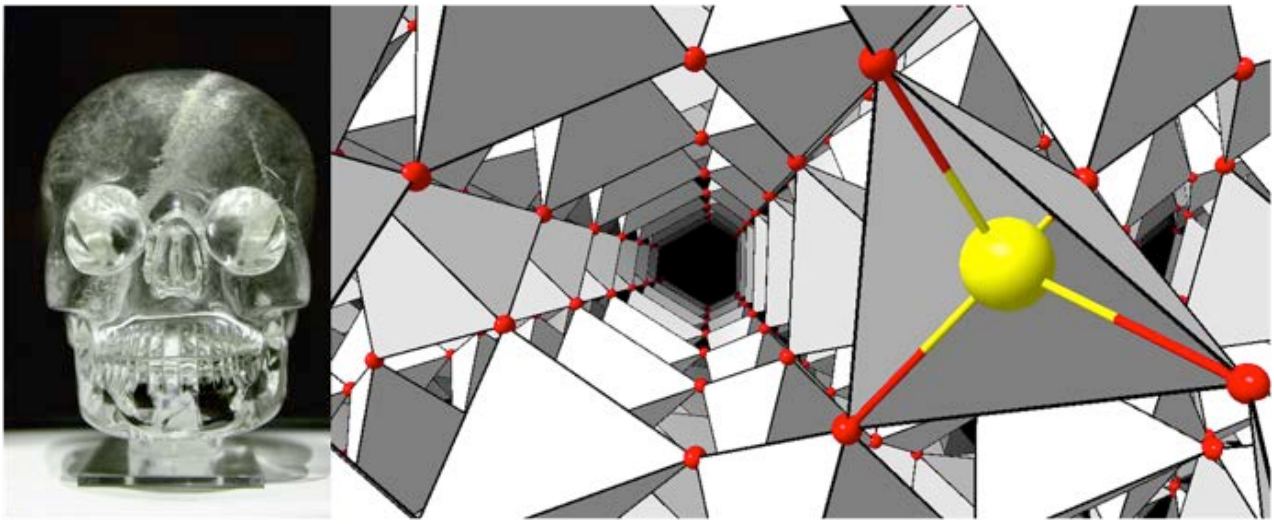
International Year of Crystallography Activities

"Crystallography365" and "Crystals in the City'

Neeraj Sharma and Helen Maynard-Casely

Two projects to celebrate International year of crystallography are being brewed up by Neeraj Sharma of UNSW and Helen Maynard-Casely of ANSTO. The first of these, led by Helen, is already up and running, Crystallography365 at http://crystallography365.wordpress.com/. This initiative will attempt to blog a crystal structure a day for all of 2014! It gathers a group of interested scientists, principally students and early career researchers, and each day during 2014 a different crystal structure will be presented and described. The goals of the project is to present to the world, the wide range of uses crystal structures have in society, the broad spectrum of sciences that rely on crystal structures, and to provide an outlet for this group of scientists to engage with the International Year of Crystallography. Have you got a structure that you'd like to share with the world? Anybody interested in writing posts for crystallography365 should get in touch with Helen (helen.maynard-casely@ansto.gov.au).

The other (hopefully bigger) project is called 'Crystals in the City'. This project is scheduled to run between the 9th-30th August 2014 (coinciding with National Science Week in Australia). This will encompass a public display of 10-15 person-size crystal structure models exhibited in various locations in cities around Australia. The goal is that the crystal structures will 'reflect' their surroundings and instil pride among the public in the crystallographic achievements of Australian science. The crystal structures will focus on the contribution Australian science has made to their use or development. Plans are afoot to have displays and temporary hands-on activities near the crystal structures for selected periods in National Science Week and an opening event to be held in conjunction with an exhibition organised by A/Prof. Chris Ling at the Verge Gallery at the University of Sydney. Accompanying the exhibition will be a website, where the public can find more about each of the structures and students can learn of opportunities to study crystallography. It will be a longer-term resource targeted to students who have an interest in crystallography or who require assistance in crystallography during their studies. The project will attempt to unite a host of supporters and sponsors; universities, museums and crystallographic groups.

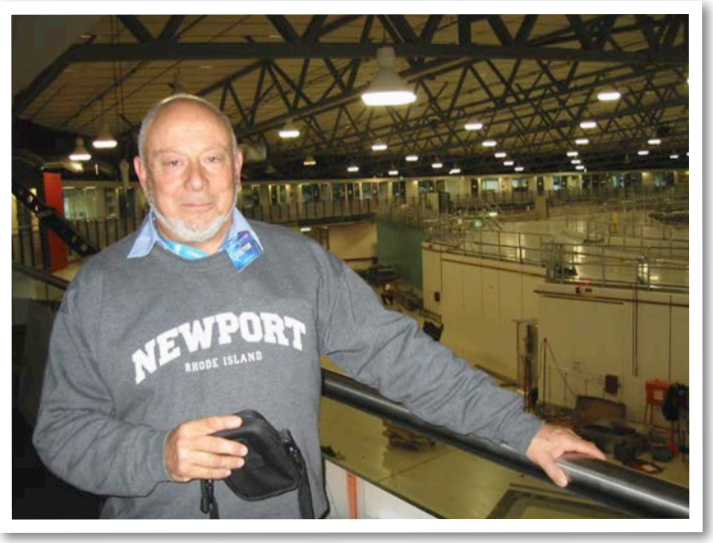


Left, Crystal skull from the British Museum - picture taken by Rafal Chalgasiewicz.
Right, the crystal structure of quartz, representation was generated using Diamond http://www.crystalimpact.com/diamond/. These are images are from Hubert Chevreau's post on Quartz, read this post here http://crystallography365.wordpress.com/2014/01/14/quartz-dear-indi-let-me-in-next-time/

TRIBUTE

Steve Wilkins (1946–2013)

by Jose Varghese



The passing of Steve Wilkins, an enduring and endearing figure in the crystallographic community, was met with shock and disbelief. He died while doing what he loved best, teaching a new generation of students at Monash University the science of X-rays.

We met as PhD students in the early '70s, at one of the bush crystallography meetings in Adelaide. He carried out his PhD under Professor J. M. Cowley, working in the area of diffuse scattering from alloys and the role of long-range interactions. His PhD thesis was entitled Correlations and Interactions in Binary Alloys. From 1970 to 1971, during his PhD, he worked as a graduate research assistant in the Department of Physics, Arizona State University. He joined CSIRO, Division of Chemical Physics, in 1975 as a Research Scientist and was promoted to Chief Research Scientist in 1998. At CSIRO he worked on a range of theoretical problems in X-ray crystallography, including quantum effects in the theory of atomic vibrations, the role of asymmetry in the problem of multiple scattering (also called 'extinction') in structure determination from crystals, and also new approaches to the determination of the atomic structure of molecules from structure- factor magnitudes (also called the 'phase problem'). I collaborated with him on the latter, work which rested on a powerful and very general branch of statistical inference known as 'information theory', which has the maximum-entropy method as a cornerstone. The work helped to advance this methodology into the mainstream of crystallography where, when combined with Bayesian methods, it has now become a very powerful technique for the structure determination of macromolecules, particularly in combination with multiple-wavelength anomalous diffraction (MAD) data.

As a result of a serendipitous encounter at the International Union of Crystallography Congress in Hamburg in 1984 with Professor Jimpei Harada, his former lecturer from his Melbourne University days (by then at Nagoya University), Steve Wilkins was invited to visit Japan the following year to explore possibilities for Australian collaboration with the newly established synchrotron in Japan known as the Photon Factory. The resulting visit (which took place in November 1985 and was funded by the Japanese Society

Tribute

Steve Wilkins (1946-2013)

for Promotion of Science) led to a formal invitation for Australia to build and operate a beamline at the Photon Factory. Following much lobbying of the government and the local scientific community, a multi-purpose powder diffractometer (called 'BigDiff'), conceived by Steve Wilkins, was built at CSIRO in Clayton under his guidance. It was installed at the Photon Factory and started operation in 1992 as the Australian National Beamline Facility (ANBF). It has only just been decommissioned and is now at the Australian Synchrotron where it will go on display. During the construction of BigDiff, I worked with Steve on adapting the instrument to protein crystallography and modification of the X-ray optics at the ANBF. We also worked closely on the Australian Synchrotron proposal, lobbying both federal and state governments and professional societies, he concentrating on the physics applications and I on the biological applications. Later we worked together on the National Scientific Advisory Committee and chaired some of the Beamline Advisory Panels that were responsible for the development of the Australian Synchrotron and the beamlines. He championed the Medical Imaging Beamline and was one of the driving forces behind its development.

Steve with his mentor Sandy Mathieson

Steve and his co-workers also worked on hard X-ray phase- contrast imaging, where they made seminal and pioneering contributions including the development of related practical methods and instruments that can use conventional ('poly- chromatic') X-ray sources. This opened the way for the widespread implementation of hard X-ray phase-contrast imaging in research, and increasingly in industry and medicine. When the CSIRO P-Health Flagship was initiated, Steve was the Leader in X-ray imaging and one of his projects to use synchrotron X-ray methods for determining the number of plaques in the brains of Alzheimer's sufferers is still being pursued.

Steve was a tireless worker for SCANZ and the Australian Academy's National Committee for Crystallography. In his quietly efficient way, he organized many meetings for the community, and while he was President of SCANZ he lobbied for SCANZ to organize the Bragg Centennial in December 2012. This meeting was coordinated to be held in conjunction with the SCANZ and the Asian Crystallography Association meetings and was an immensely successful event. He organized the Bragg Centennial Symposium, inviting several notable crystallographers who were connected to Lawrence Bragg, as well as members of the Bragg family.

Steve exemplified the quiet achiever and was able to overcome considerable hurdles in seeking the goals he set his eyes on, by a quiet confidence, a sharp intellect and persuasive arguments. He was a scholar and a gentleman, and the crystallographic community shall miss him.

Steve and team receiving the CSIRO Medal (1998) for the development of phase-contrast X-ray imaging methods using laboratory-based microfocus sources. From left to right, Andrew Stevenson, Tim Gureyev, Steve, Andrew Pogany, Dachao Gao, and Tim Davis.

Steve and Jose

Special thanks to Andrew Stevenson for pictures

TRIBUTE

"Blue" Barclay (1923–2013)

by Colin Kennard

It was with great sadness when I read in Saturday 4th January 2014 Sydney Morning Herald Obituary section about the death of my Ph.D. supervisor, Blue Barclay.

At the end of 1957, after two years in industry and with a Bachelor of Science in Applied Chemistry from the then New South Wales University of Technology in Ultimo, I decided to see if I was eligible for a higher degree. Blue interviewed me and signed me up for a Doctor of Philosophy degree in "crystallography". I was, I think, Blue's first graduate student. In 1958, I took a whole year to determine the structure of a four atom problem [G.A. Barclay and C.H.L. Kennard, "The Crystal Structure of Anhydrous Copper(II) Formate", J.Chem.Soc., 3289-3294,(1961)], taking X-ray photographs, estimating intensities by eye, and using a noisy Madas calculator solving the vector Patterson, calculating Structure Factors, and with Beer-Lipson strips calculating a Fourier synthesis and repeating this process until refinement was achieved. Today this would be a two hour student practical exercise.

In 1959, I graduated to use NSWUT Utecom [Deuce] computer which was housed in the basement of the then Physics building at the old racecourse at Kensington. Monday night was our computing night, and Blue and I would have a game of Squash after my six hour demonstrating day, then an evening meal and start on Utecom by 7. Blue would stay with me until about 11.00 that night, and I would keep computing until I was thrown out at 8 the following morning. I did this for two years. This type of work is now easily performed on a laptop. At this stage of Blue's life, he was an administrator and as we did not have a least squares refinement program set himself a challenge to write in machine language a differential synthesis which could run on this 1.6KB mercury memory computer with 1450 thermionic valves. This worked well.

I finished in 1960, and graduated the following year. I did four years post doctoral research at Cornell University. Ithaca, New York and the University of Washington, Seattle, Washington. I returned to Australia in 1964 with a lecturing position at the University of Queensland until I retired in 1999.

Looking back, Blue played a major role in my early life and he was an excellent supervisor. I can't comment on whether I was a good graduate student, but we worked hard, put in long hours and got rewards. Thanks Blue.

Upcoming Meetings

Crystal 29 Conference, 22-25 April 2014